The Independence on Boundary Conditions for the Thermodynamic Limit of Charged Systems *

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Abstract

We study systems containing electrons and nuclei. Based on the fact that the Thermodynamic limit exists for systems with Dirichlet boundary conditions, we prove that the same limit is obtained if one imposes other boundary conditions such as Neumann, periodic, or elastic boundary conditions. The result is proven for all limiting sequences of domains which are obtained by scaling a bounded open set, with smooth boundary, except for isolated edges and corners.

1 Introduction

We consider systems composed of electrons and nuclei, i.e., point particles which interact via Coulomb interaction with the negatively charged particles being fermions. Due to their important role in describing nature, such systems have been intensively investigated. In particular, the thermodynamic limit, i.e., the limit in which the system becomes large, has been studied extensively in [1]. In that work, it was shown that the thermodynamic limit exists for thermodynamic quantities, such as the pressure and the free energy density, provided that they are defined using Dirichlet boundary conditions. Furthermore, it was shown that these quantities possess the properties which are expected from phenomenological thermodynamics.

In order to define the canonical and the grand canonical partition function, one has to confine the particles of the system to lie in a bounded set $\Lambda \subset \mathbb{R}^3$, which we choose to be open. For the confined system to be well defined its Hamiltonian should be self adjoint. This requires that one imposes suitable boundary conditions on the boundary of Λ. For each particular choice of boundary conditions one obtains a canonical and a grand canonical partition function. In order to study the thermodynamic limit one considers

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a sequence $\{\Lambda_l\}$ of bounded open domains such that the volume of Λ_l tends to infinity as $l \to \infty$. For systems with Dirichlet boundary conditions it was shown in [1] that the canonical and grand canonical partition function exist for a large class of limiting sequences $\{\Lambda_l\}$. Moreover, the limit is independent of the particular sequence.

In this work we prove that, indeed, the same limit is obtained for systems with Neumann, periodic, or reflecting boundary conditions. We prove our result for limiting sequences which are obtained by scaling a bounded open set, which has a smooth boundary, except for isolated edges and corners. This class of limiting sequences is smaller than the class for which the thermodynamic limit for systems with Dirichlet boundary conditions has been shown to exist. We want to point out that this is only partially technical. For instance, there exist sequences of domains for which the thermodynamic limit of the ground state energy for Dirichlet boundary conditions exists, whereas for Neumann boundary conditions the ground state energy diverges to $-\infty$. Although such sequences are somewhat pathological, this demonstrates that the independence of boundary conditions for systems composed of electrons and nuclei cannot be considered as trivial. We will also comment on possible more general classes of limiting sequences for which our proof is applicable. For notational simplicity, we only state and prove our results for systems composed of a single species of negatively charged fermions and a single species of positively charged particles being bosons. The results as well as their proofs generalize to multicomponent systems in a straight forward way. We state the main result and present its proof for both: zero temperature and nonnegative temperature. Despite that the latter implies the former, we present that way an independent and technically easier proof for the temperature zero case.

To prove the independence of the boundary conditions we use a sliding technique, which was introduced in [2], and refined in [3]. Thereby, one decomposes the space into simplices. By sliding and rotating the simplices one obtains a lower bound for the Hamiltonian of a large system in terms of Hamiltonians defined on the smaller simplices. Simplices which lie in the interior of the large system have Dirichlet boundary conditions. Whereas simplices on the boundary, i.e., simplices which intersect with the boundary of the large system, are subject to mixed boundary conditions. Using that the many body Coulomb potential can be estimated below by a sum of one body potentials [8], we then show that the thermodynamic quantities in the boundary simplices are bounded. In the thermodynamic limit the sum of all the boundary contributions is proportional to the surface. This is negligible compared to the bulk contribution, which is proportional to the volume.

We want to point out that independence of boundary conditions has been studied for systems with hard core interactions (see [4], [5], and references given therein).

The paper is organized as follows. In Section 2 we introduce the model and state the results. In section 3 we present the proofs.

2 Model and Statement of Results

We shall first recall the definition of Dirichlet and Neumann boundary conditions [6]. Let Λ be a bounded open set in $\mathbb{R}^3$. The Dirichlet Laplacian for Λ, $-\Delta_\Lambda^{\mathrm{D}}$, is the unique

self-adjoint operator on $L^2(\Lambda)$ whose quadratic form is the closure of the form

$$\phi \mapsto \int_\Lambda |\nabla\phi|^2 \, dx$$

with domain $C_0^\infty(\Lambda)$. The Neumann Laplacian for Λ, $-\Delta_\Lambda^{\mathrm{N}}$, is the unique self-adjoint operator on $L^2(\Lambda)$ whose quadratic form is

$$\phi \mapsto \int_\Lambda |\nabla\phi|^2 \, dx$$

with domain $H^1(\Lambda) = \{\ f \in L^2(\Lambda) \mid \nabla f \in L^2(\Lambda) \text{ (in sense of distributions) } \}$.

The model consists of electrons ($\hbar^2/2 = 1$, $m = 1$, $|e| = 1$) and nuclei with mass M and charge z. We assume z to be rational. The electrons are fermions, while the statistics of the nuclei is irrelevant. Let $\Lambda \in \mathbb{R}^3$ be an open set. The Hilbert space $\mathcal{H}_{\boldsymbol{N},\Lambda}$, with $\boldsymbol{N} = (n, k) \in \mathbb{N}^2$, for n electrons and k nuclei is the subspace of $L^2(\Lambda \times \mathbb{Z}_2)^{\otimes n} \otimes L^2(\Lambda)^{\otimes k}$ carrying the permutation symmetry appropriate to the given statistics. The Hamiltonian, acting on $\mathcal{H}_{\boldsymbol{N},\Lambda}$, is

$$\begin{aligned} H^B_{\boldsymbol{N},\Lambda} &= -\sum_{j=1}^{n} \Delta^B_{\Lambda,x_j} - \frac{1}{M}\sum_{j=1}^{k} \Delta^B_{\Lambda,R_j} - z\sum_{i=1}^{n}\sum_{j=1}^{k} \frac{1}{|x_i - R_j|} \\ &\quad + \sum_{1\le i<j\le n} \frac{1}{|x_i - x_j|} + z^2 \sum_{1\le i<j\le k} \frac{1}{|R_i - R_j|} \, , \end{aligned}$$

where the electron coordinates are x_i, the nuclear coordinates are R_i and by B we denote the type of boundary conditions, e.g. N, D, and M stands for Neumann, Dirichlet, and mixed boundary conditions. Variable particle numbers are accounted for by means of the direct sum

$$\mathcal{H}_\Lambda = \bigoplus_{\boldsymbol{N}} \mathcal{H}_{\boldsymbol{N},\Lambda} \quad , \qquad H^B_\Lambda = \bigoplus_{\boldsymbol{N}} H^B_{\boldsymbol{N},\Lambda} \, . \tag{1}$$

The grand canonical partition function and the (finite volume) pressure are defined by

$$\begin{aligned} \Xi^B(\beta, \boldsymbol{\mu}, \Lambda) &= \mathrm{Tr}_{\mathcal{H}_\Lambda}\, e^{-\beta(H^B_\Lambda - \boldsymbol{\mu}\cdot\boldsymbol{N})} = \sum_{\boldsymbol{N}} \mathrm{Tr}_{\mathcal{H}_{\boldsymbol{N},\Lambda}}\, e^{-\beta(H^B_{\boldsymbol{N},\Lambda} - \boldsymbol{\mu}\cdot\boldsymbol{N})} \\ p^B(\beta, \boldsymbol{\mu}, \Lambda) &= (\beta|\Lambda|)^{-1} \log \Xi^B(\beta, \boldsymbol{\mu}, \Lambda) \, , \end{aligned}$$

where $\boldsymbol{\mu} = (\mu_n, \mu_k) \in \mathbb{R}^2$ stands for the chemical potentials of the electrons and the nuclei, $\beta > 0$ is the inverse temperature, and $\boldsymbol{N}$ denotes the particle number operator, for which we use the same symbol as for its eigenvalues. Here and below the volume of a subset Ω in $\mathbb{R}^3$ is denoted by $|\Omega|$. The canonical partition function of the system at reciprocal temperature β and the free energy per unit volume are defined by

$$\begin{aligned} Z^B(\beta, \boldsymbol{N}, \Lambda) &= \mathrm{Tr}_{\mathcal{H}_{\boldsymbol{N},\Lambda}}\, e^{-\beta H^B_{\boldsymbol{N},\Lambda}} \\ f^B(\beta, \boldsymbol{N}, \Lambda) &= -(\beta|\Lambda|)^{-1} \log Z^B(\beta, \boldsymbol{N}, \Lambda) \, . \end{aligned}$$

Furthermore, we consider the following zero temperature expressions, which we will denote as

$$G^B(\boldsymbol{\mu},\Lambda) = \inf \sigma_{\mathcal{H}_\Lambda}(H^B_\Lambda - \boldsymbol{\mu}\cdot\boldsymbol{N}) \ , \quad g^B(\boldsymbol{\mu},\Lambda) = \frac{1}{|\Lambda|} G^B(\boldsymbol{\mu},\Lambda) \ ,$$

$$E^B(\boldsymbol{N},\Lambda) = \inf \sigma_{\mathcal{H}_\Lambda}(H^B_{\boldsymbol{N},\Lambda}) \ , \quad e^B(\boldsymbol{N},\Lambda) = \frac{1}{|\Lambda|} E^B(\boldsymbol{N},\Lambda) \ .$$

Definition 1. *A sequence $\{\Lambda_l\}$ of bounded open sets in $\mathbb{R}^3$ is called a regular sequence of domains if:*

(i) *For $l \to \infty$, $|\Lambda_l| \to \infty$.*

(ii) *For each fixed $h \geq 0$ as $l \to \infty$ (with $\Lambda_l^c = \mathbb{R}^3 \setminus \Lambda_l$)* $|\{ \ x \in \Lambda_l \mid d(x, \Lambda_l^c) < h \ \}|/|\Lambda_l| \to 0$ *and* $|\{ \ x \in \Lambda_l^c \mid d(x, \Lambda_l) \leq h \ \}|/|\Lambda_l| \to 0$.

(iii) *There exists a $\delta > 0$ such that for all l, $|\Lambda_l|/|B_l| \geq \delta$, where B_l is the ball of smallest radius containing Λ_l.*

It was shown in [1] that for regular sequences $\{\Lambda_l\}$ the thermodynamic limits

$$p^{\mathrm{D}}(\beta,\boldsymbol{\mu}) = \lim_{l\to\infty} p^{\mathrm{D}}(\beta,\boldsymbol{\mu},\Lambda_l) \ , \qquad \lim_{l\to\infty} g^{\mathrm{D}}(\boldsymbol{\mu},\Lambda_l) = g^{\mathrm{D}}(\boldsymbol{\mu})$$

for Dirichlet boundary conditions exist and are independent of the particular sequence. To study the thermodynamic limit for the canonical ensemble, we consider systems with no net charge, i.e.,

$$\boldsymbol{N} = (n,k) \ \text{ with } \quad k = zn \ .$$

We introduce the set

$$P_S = \{ \ (\rho_e, \rho_k,) \in \mathbb{R}^2_+ \mid \rho_k = z\rho_e \ \} \ ,$$

corresponding to neutral charge configurations. In [1], it was also shown that for a regular sequence of domains $\{\Lambda_l\}$ and neutral $\{\boldsymbol{N}_l\}$, i.e., $\boldsymbol{N}_l \in \mathbb{N}^2 \cap P_S$, with

$$\lim_{l\to\infty} \frac{\boldsymbol{N}_l}{|\Lambda_l|} = \boldsymbol{\rho} \equiv (\rho_e, \rho_k) \in P_S \ ,$$

the limits for Dirichlet conditions

$$\lim_{l\to\infty} f^{\mathrm{D}}(\beta, \boldsymbol{N}_l, \Lambda_l) = f^{\mathrm{D}}(\beta,\boldsymbol{\rho}) \ , \qquad \lim_{l\to\infty} e^{\mathrm{D}}(\boldsymbol{N}_l,\Lambda_l) = e^{\mathrm{D}}(\boldsymbol{\rho})$$

exist independent of the particular sequence and are convex functions of $\boldsymbol{\rho} \in P_S$. The value of $\boldsymbol{\rho}$ gives the density of the particles. Furthermore, it was shown that the canonical and the grand canonical ensembles are equivalent, i.e., that

$$p^{\mathrm{D}}(\beta,\boldsymbol{\mu}) = \sup_{\boldsymbol{\rho}\in P_S} (\boldsymbol{\rho}\cdot\boldsymbol{\mu} - f^{\mathrm{D}}(\beta,\boldsymbol{\rho})) \ , \qquad g^{\mathrm{D}}(\boldsymbol{\mu}) = \inf{}_{\boldsymbol{\rho}\in P_S} (e^{\mathrm{D}}(\boldsymbol{\rho}) - \boldsymbol{\mu}\cdot\boldsymbol{\rho}) \ . \qquad (2)$$

We note that (2) implies that $g^{\mathrm{D}}(\boldsymbol{\mu})$ is concave and that $p^{\mathrm{D}}(\beta,\boldsymbol{\mu})$ is convex, and hence they are continuous functions of $\boldsymbol{\mu}$. We now state our main result.

Theorem 1. *Let $\Lambda \subset \mathbb{R}^3$ be a bounded open set with smooth boundary, except for isolated edges and corners. Consider the sequence $\Lambda_L = L\Lambda$ for $L > 0$. Then*

(a) $g^{\mathrm{N}}(\boldsymbol{\mu}) = \lim_{L\to\infty} |\Lambda_L|^{-1} G^{\mathrm{N}}(\boldsymbol{\mu}, \Lambda_L) = g^{\mathrm{D}}(\boldsymbol{\mu})$.

(b) $p^{\mathrm{N}}(\beta, \boldsymbol{\mu}) = \lim_{L\to\infty} p^{\mathrm{N}}(\beta, \boldsymbol{\mu}, \Lambda_L) = p^{\mathrm{D}}(\beta, \boldsymbol{\mu})$.

We want to point out that sequences satisfying the assumption of Theorem 1 are regular sequences of domains. Theorem 1 has the following consequence.

Corollary 2. *Let $\{\Lambda_L\}$ be a sequence of domains as in Theorem 1. Let $\{\boldsymbol{N}_L\}$ be a sequence with neutral charge configuration, i.e., $\boldsymbol{N}_L \in \mathbb{N}^2 \cap P_S$, such that*

$$\lim_{L\to\infty} \frac{\boldsymbol{N}_L}{|\Lambda_L|} = \boldsymbol{\rho} \in P_S \ .$$

Then

(a) $e^{\mathrm{N}}(\boldsymbol{\rho}) := \lim_{L\to\infty} e^{\mathrm{N}}(\boldsymbol{N}_L, \Lambda_L) = e^{\mathrm{D}}(\boldsymbol{\rho})$;

(b) $f^{\mathrm{N}}(\beta, \boldsymbol{\rho}) := \lim_{L\to\infty} f^{\mathrm{N}}(\beta, \boldsymbol{N}_L, \Lambda_L) = f^{\mathrm{D}}(\beta, \boldsymbol{\rho})$.

Remark 1. Note that we only consider systems which consist of electrons and one type of spinless nuclei. The results and their proofs generalize in a straight forward way to multicomponent systems, with all negatively (or positively) charged particles being fermions.

Remark 2. The essential technical requirement in the proof of Theorem 1 on the sequence of domains Λ_L, apart from being regular, is that the thermodynamic quantities of the boundary simplices are bounded, cp. Lemma 5. This in turn holds for all sequences satisfying the assertion of Lemma 7, which is stated in the next section. We want to point out that there do exist sequences of domains for which the thermodynamic limit does not exist for systems with Neumann boundary conditions, and yet for Dirichlet conditions the thermodynamic limit exists, cp. the example below.

Example 1. We consider a system where the charge z of the nuclei is one. Let $\{\Lambda_l\}$ be the union of a large ball B_l of radius l and a shrinking ball $B_{l^{-4}}$ of radius l^{-4} separated from the large ball by a constant distance. Let $\{\boldsymbol{N}_l\}$ be a sequence with $\boldsymbol{N}_l \in \mathbb{N}^2 \cap P_S$ $\lim_{l\to\infty} |\Lambda_l|^{-1}\boldsymbol{N}_l = \boldsymbol{\rho}$. The sequence $\{\Lambda_l\}$ is a regular sequence of domains. We place one electron and a single nucleus in the small ball and put both in the Neumann ground state. In that situation the small ball has neutral charge distribution and hence there is no Coulomb interaction with the large ball. This provides us with the following upper bound

$$e^{\mathrm{N}}(\Lambda_l, \boldsymbol{N}_l) \leq |\Lambda_l|^{-1} E^{\mathrm{D}}(B_l, \boldsymbol{N}_l - (1,1)) + |\Lambda_l|^{-1} |B_{l^{-4}}|^{-2} \int_{(B_{l^{-4}})^2} \frac{-1}{|x-y|}\, dxdy \ .$$

The first term on the right hand side converges to $e^{\mathrm{D}}(\boldsymbol{\rho})$ while the second term diverges to $-\infty$. The same conclusion is easily seen to hold if we connect the small ball to the large ball by a thin tube provided that its thickness shrinks fast enough.

Finally we want to consider more general boundary conditions. Consider for instance, a Laplacian $-\Delta_\Lambda^{\mathrm{A}}$ with boundary conditions such that

$$-\Delta_\Lambda^{\mathrm{N}} \leq -\Delta_\Lambda^{\mathrm{A}} \leq -\Delta_\Lambda^{\mathrm{D}} \; . \tag{3}$$

(Here and below operator inequalities are understood in the sense of forms [6].) Then Theorem 1 and Corollary 2, respectively, imply that the same limits are obtained for systems with boundary conditions satisfying (3). We note that periodic boundary conditions are of this type.

Elastic boundary conditions, with elasticity σ, are defined as follows. Let t_Λ^σ denote the quadratic form which is the closure of the form

$$\phi \mapsto \int_\Lambda |\nabla\phi|^2 \, dx + \sigma \int_{\partial\Lambda} |\phi|^2 \, dS$$

with domain $H^1(\Lambda) \cap C(\overline{\Lambda})$ and where dS is the surface measure of $\partial\Lambda$, the boundary of Λ. Let $-\Delta_\Lambda^\sigma$ denote the unique self adjoint operator with quadratic form t_Λ^σ. Functions in the domain of $-\Delta_\Lambda^\sigma$ satisfy

$$\frac{\partial\phi}{\partial n} = \sigma\phi\Big|_{\partial\Lambda}$$

at the boundary of Λ, where $\partial\phi/\partial n$ denotes the normal derivative. Note that boundary conditions with elasticity zero are Neumann boundary conditions. For positive elasticity, $\sigma > 0$, we have the operator inequality $-\Delta_\Lambda^{\mathrm{N}} \leq -\Delta_\Lambda^\sigma \leq -\Delta_\Lambda^{\mathrm{D}}$. This implies the statement of the following theorem in the case where the elasticity is positive. That it, indeed, holds for negative elasticity will be shown in Section 3.4.

Theorem 3. *Let Λ_L be as in Theorem 1. Then, for elastic boundary conditions with real elasticity σ, $\lim_{L\to\infty} p^\sigma(\beta, \boldsymbol{\mu}, \Lambda_L) = p^{\mathrm{D}}(\beta, \boldsymbol{\mu})$. Let $\{\boldsymbol{N}_L\}$ be a sequence as in Corollary 2. Then $\lim_{L\to\infty} f^\sigma(\beta, \boldsymbol{N}_L, \Lambda_L) = f^{\mathrm{D}}(\beta, \boldsymbol{\rho})$.*

3 Proofs

First we show that Corollary 2 follows from Theorem 1. In subsection 3.2 we will prove Theorem 1, which is our main result. The prove is based on a lemma which estimates the contributions from the boundary terms. The prove of that lemma is deferred to subsection 3.3. In subsection 3.4 we prove Theorem 3 concerning reflecting boundary conditions.

3.1 Proof of Corollary 2

(a). We know that for $\boldsymbol{\rho} \in P_S$

$$e^{\mathrm{D}}(\boldsymbol{\rho}) \geq \liminf_{L\to\infty} e^{\mathrm{N}}(\boldsymbol{N}_L, \Lambda_L) \; . \tag{4}$$

For a given $\boldsymbol{\rho} \in P_S$ there exists, by the convexity of e^{D}, a $\boldsymbol{\mu}$ such that

$$e^{\mathrm{D}}(\boldsymbol{\rho}') \geq e^{\mathrm{D}}(\boldsymbol{\rho}) + \boldsymbol{\mu} \cdot (\boldsymbol{\rho}' - \boldsymbol{\rho}) \quad , \quad \text{for all } \boldsymbol{\rho}' \in P_S \; .$$

Hence

$$\inf_{\boldsymbol{\rho}'\in P_S}(e^{\mathrm{D}}(\boldsymbol{\rho}') - \boldsymbol{\mu}\cdot\boldsymbol{\rho}') = e^{\mathrm{D}}(\boldsymbol{\rho}) - \boldsymbol{\mu}\cdot\boldsymbol{\rho}\ . \tag{5}$$

We have

$$\begin{aligned}
\liminf_{L\to\infty} e^{\mathrm{N}}(\boldsymbol{N}_L,\Lambda_L) &= \liminf_{L\to\infty} \frac{E^{\mathrm{N}}(\boldsymbol{N}_L,\Lambda_L)}{|\Lambda_L|} \\
&= \liminf_{L\to\infty} \frac{E^{\mathrm{N}}(\boldsymbol{N}_L,\Lambda_L) - \boldsymbol{\mu}\cdot\boldsymbol{N}_L}{|\Lambda_L|} + \boldsymbol{\mu}\cdot\boldsymbol{\rho} \\
&\geq \liminf_{L\to\infty} \left(\inf_{\boldsymbol{N}} \frac{E^{\mathrm{N}}(\boldsymbol{N},\Lambda_L) - \boldsymbol{\mu}\cdot\boldsymbol{N}}{|\Lambda_L|}\right) + \boldsymbol{\mu}\cdot\boldsymbol{\rho} \\
&= g^{\mathrm{D}}(\boldsymbol{\mu}) + \boldsymbol{\mu}\cdot\boldsymbol{\rho} \\
&= \inf_{\boldsymbol{\rho}'\in P_S}(e^{\mathrm{D}}(\boldsymbol{\rho}') - \boldsymbol{\mu}\cdot\boldsymbol{\rho}') + \boldsymbol{\mu}\cdot\boldsymbol{\rho} \\
&= e^{\mathrm{D}}(\boldsymbol{\rho})\ ,
\end{aligned}$$

where we have used Theorem 1 (a) in the fourth, eq. (2) in the fifth and eq. (5) in the last line. The above inequality together with (4) proves (a).

(b). The proof of (b) is analogous to (a). We know that for $\boldsymbol{\rho}\in P_S$

$$-f^{\mathrm{D}}(\beta,\boldsymbol{\rho}) \leq \limsup_{L\to\infty}(-f^{\mathrm{N}}(\beta,\boldsymbol{N}_L,\Lambda_L))\ , \tag{6}$$

where we used that the map $A\mapsto \operatorname{Tr} e^A$ is operator monotone. Since $P_S\ni\boldsymbol{\rho}\mapsto -f^{\mathrm{D}}(\beta,\boldsymbol{\rho})$ is concave, there exists for a given $\boldsymbol{\rho}\in P_S$ a $\boldsymbol{\mu}$ such that

$$-f^{\mathrm{D}}(\beta,\boldsymbol{\rho}') \leq -f^{\mathrm{D}}(\beta,\boldsymbol{\rho}) - \boldsymbol{\mu}\cdot(\boldsymbol{\rho}'-\boldsymbol{\rho})\quad ,\quad \text{for all } \boldsymbol{\rho}'\in P_S\ ,$$

and hence

$$\sup_{\boldsymbol{\rho}'\in P_S}\left(\boldsymbol{\rho}'\cdot\boldsymbol{\mu} - f^{\mathrm{D}}(\beta,\boldsymbol{\rho}')\right) = \boldsymbol{\rho}\cdot\boldsymbol{\mu} - f^{\mathrm{D}}(\beta,\boldsymbol{\rho})\ . \tag{7}$$

We have

$$\begin{aligned}
&\limsup_{L\to\infty}\left(-f^{\mathrm{N}}(\beta,\boldsymbol{N}_L,\Lambda_L)\right) = \\
&\quad = \limsup_{L\to\infty}\left(-\boldsymbol{\rho}\cdot\boldsymbol{\mu} + (\beta|\Lambda_L|)^{-1}\beta\boldsymbol{\mu}\cdot\boldsymbol{N}_L - f^{\mathrm{N}}(\beta,\boldsymbol{N}_L,\Lambda_L)\right) \\
&\quad = -\boldsymbol{\rho}\cdot\boldsymbol{\mu} + \limsup_{L\to\infty}\left((\beta|\Lambda_L|)^{-1}\log Z^{\mathrm{N}}(\beta,\boldsymbol{N}_L,\Lambda_L)e^{\beta\boldsymbol{\mu}\cdot\boldsymbol{N}_L}\right) \\
&\quad \leq -\boldsymbol{\rho}\cdot\boldsymbol{\mu} + \limsup_{L\to\infty}\left((\beta|\Lambda_L|)^{-1}\log\left(\sum_{\boldsymbol{N}} Z^{\mathrm{N}}(\beta,\boldsymbol{N},\Lambda_L)e^{\beta\boldsymbol{\mu}\cdot\boldsymbol{N}}\right)\right) \\
&\quad = -\boldsymbol{\rho}\cdot\boldsymbol{\mu} + p^{\mathrm{D}}(\beta,\boldsymbol{\mu}) \\
&\quad = -f^{\mathrm{D}}(\beta,\boldsymbol{\rho})\ ,
\end{aligned}$$

where we have used Theorem 1 (b) in the fourth and eqns. (2,7) in the last line. The above inequality together with (6) proves (b). □

3.2 Proof of Theorem 1

To prove Theorem 1, we will make use of the localization method of [3] (see also [2]), where one breaks up $\mathbb{R}^3$ into simplices in the following way. Cutting the unit cube $W = [0,1]^3$ with all planes passing through the centre and an edge or a face diagonal of W, one obtains congruent simplices $\triangle_n \subset W$, $(n = 1, ..., 24)$. The simplices $\triangle_\alpha = \triangle_n + z$, with $\alpha = (z, n) \in \mathbb{Z}^3 \times \{1, ..., 24\} =: I$, yield a partition of $\mathbb{R}^3$ up to their boundaries. We then choose a spherically symmetric $\varphi_0 \in C_0^\infty(\mathbb{R}^3)$ with $\int \varphi_0^2 = 1$ and $\{\varphi_0(x) \neq 0\} = \{|x| < 1/2\}$. Let χ_α be the characteristic function of $\triangle_\alpha$. Setting $\varphi(x) = \eta^{-3/2}\varphi_0(x/\eta)$ and $j_\alpha = (\chi_\alpha * \varphi^2)^{1/2}$, we obtain a partition of unity, i.e.,

$$\sum_{\alpha \in I} j_\alpha^2(x) = 1 \quad , \ (x \in \mathbb{R}^3) \ ,$$

with $j_\alpha \in C^\infty(\mathbb{R}^3)$. There are congruent simplices $\triangle_\alpha^+$, which are scaled copies of $\triangle_\alpha$, such that

$$\begin{aligned} \operatorname{supp} j_\alpha &\subset \triangle_\alpha^+ \\ |\triangle_\alpha^+| &\leq |\triangle_\alpha|(1 + O(\eta)) \end{aligned}$$

as $\eta \downarrow 0$.

The following definitions depend on η and $l > 0$ although the notation will not reflect this for simplicity. For the moment, let $\Lambda \subset \mathbb{R}^3$ be any bounded open set. For $y \in W$ and $R \in SO(3)$ we set

$$\Lambda^{y,R} = R^{-1}\Lambda - ly \ .$$

We define the set

$$I(\Lambda) = \{\alpha \in I | l\triangle_\alpha^+ \cap \Lambda^{y,R} \neq \emptyset \text{ for some } y \in W, R \in SO(3)\} \ .$$

For $\alpha \in I(\Lambda)$, let $\mathcal{H}_\alpha := \mathcal{H}_{l\triangle_\alpha^+}$ be the many particle space for the simplices $l\triangle_\alpha^+$ as given in (1). By $H^{\mathrm{M}}_{\alpha,y,R,\Lambda}$ we denote the Hamiltonian on $l\triangle_\alpha^+ \cap \Lambda^{y,R}$ with Neumann conditions on $(l\triangle_\alpha^+) \cap \partial\Lambda^{y,R}$ and Dirichlet conditions on the remaining part of the boundary. The operator $H^{\mathrm{M}}_{\alpha,y,R,\Lambda}$ acts on

$$\mathcal{H}_{\alpha,y,R,\Lambda} := \mathcal{H}_{l\triangle_\alpha^+ \cap \Lambda^{y,R}} \hookrightarrow \mathcal{H}_\alpha$$

and hence on $\mathcal{H}_\alpha$ via the canonical embedding. Note, if $l\triangle_\alpha^+ \subset \Lambda^{y,R}$, then $H^{\mathrm{M}}_{\alpha,y,R,\Lambda} = H^{\mathrm{D}}_{l\triangle_\alpha^+}$ and $\mathcal{H}_{\alpha,y,R,\Lambda} = \mathcal{H}_\alpha$. We define the Hilbert space and a Hamiltonian, acting on it, as the direct integrals

$$\begin{aligned} \mathcal{H}_{I(\Lambda)} &= \int_{W \times SO(3)}^{\oplus} dy d\mu(R) \bigotimes_{\alpha \in I(\Lambda)} \mathcal{H}_\alpha \ , \\ H^{\mathrm{N}}_{I(\Lambda)} &= \int_{W \times SO(3)}^{\oplus} dy d\mu(R) \sum_{\alpha \in I(\Lambda)} H^{\mathrm{M}}_{\alpha,y,R,\Lambda} \ , \end{aligned}$$

where $d\mu$ denotes the Haar measure on $SO(3)$. We shall define a map $J : \mathcal{H}_\Lambda \to \mathcal{H}_{I(\Lambda)}$ as follows. Let $j_{y,R,\alpha} : L^2(\Lambda) \to L^2(l\triangle_\alpha^+)$ be given by

$$(j_{y,R,\alpha}\psi)(x) = j_\alpha(x/l)\psi(R(x + ly)) \ .$$

Define

$$\begin{aligned} j_{y,R} : L^2(\Lambda) &\rightarrow \bigoplus_{\alpha \in I(\Lambda)} L^2(l\triangle_\alpha^+) \\ j_{y,R} &= \bigoplus_{\alpha \in I(\Lambda)} j_{y,R,\alpha} \; . \end{aligned}$$

This lifts to a map between the many particle spaces

$$\Gamma(j_{y,R}) : \mathcal{H}_\Lambda \rightarrow \bigotimes_{\alpha \in I(\Lambda)} \mathcal{H}_\alpha \; ,$$

which acts as the $\boldsymbol{N}$-fold tensor product of $j_{y,R}$ on $\boldsymbol{N}$-particle states. We may now define

$$J : \mathcal{H}_\Lambda \rightarrow \mathcal{H}_{I(\Lambda)} \; , \qquad J = \int_{W \times SO(3)}^{\oplus} dy d\mu(R) \Gamma(j_{y,R}) \; .$$

We note that the map $j^*_{y,R,\alpha} : L^2(l\triangle_\alpha^+) \rightarrow L^2(\Lambda)$ is given by

$$(j^*_{y,R,\alpha}\psi)(x) = j_\alpha(R^{-1}(x/l) - y)\psi(R^{-1}x - ly) \; .$$

Hence $j^*_{y,R} j_{y,R} : L^2(\Lambda) \rightarrow L^2(\Lambda)$ acts as multiplication by $\sum_{\alpha \in I(\Lambda)} j_\alpha^2(R^{-1}(x/l) - y)$. This function of $x \in \Lambda$ equals 1. We conclude that $J^*J = 1$, i.e., that J is an isometry. We state the following Lemma, c.f. Lemma 7 in [3].

Lemma 4. *Let $\eta = l^{-1}$. Then*

$$H_\Lambda^{\mathrm{N}} \geq \kappa J^* H^{\mathrm{N}}_{I(\Lambda)} J - l^{-1} \mathbf{const} \cdot \boldsymbol{N}$$

for large l, where $0 < \kappa \leq 1$ and $\kappa = 1 + O(l^{-1})$ as $l \rightarrow \infty$.

For the proof of this Lemma we refer the reader to the proof of Lemma 7 in [3], where the statement is for the Dirichlet Laplacian. With little modification of the proof given there one can proof Lemma 4.

From now on, let Λ be a fixed open set as in the assumption of Theorem 1, i.e., bounded with smooth boundary, except for isolated edges and corners. We will consider the sequence of scaled copies $\Lambda_L = L\Lambda$, with $L > 0$. Note that the claim of Lemma 4 of course holds for all Λ_L. Let $\triangle$ denote a simplex which is similar to one (and thus all) of the simplices $\triangle_\alpha$, i.e., equal up to dilations, translations, and rotations. By $\triangle_c$ we denote its intersection with Λ_L, i.e., $\triangle_c = \triangle \cap \Lambda_L$. Let $-\Delta^{\mathrm{M}}_{\triangle_c}$ ($H^{\mathrm{M}}_{\triangle_c}$) denote the Laplacian (Hamiltonian) on $\triangle_c$ with Neumann conditions on $\triangle \cap \partial\Lambda_L$ and Dirichlet conditions on the rest of $\partial\triangle_c$. We note that $-\Delta^{\mathrm{M}}_{\triangle_c}$ is the unique self adjoint operator on $L^2(\triangle_c)$ whose quadratic form is the closure of the form $\phi \mapsto \int_{\triangle_c} |\nabla\phi|^2 \, dx$ with domain $\{ \phi \in H^1(\triangle_c) \cap C(\overline{\triangle_c}) \,|\, \phi \text{ vanishes in a neighborhood of } \partial\triangle \cap \Lambda_L \}$.

The following Lemma whose prove will be postponed to subsection 3.3 provides us with a bound for the contributions from the boundary simplices.

Lemma 5. *Let Λ_L be a sequence of domains as in Theorem 1 and let $v > 0$. Then there exists a number L_0 and constants $C_E(\boldsymbol{\mu}, v)$ and $C_\Xi(\beta, \boldsymbol{\mu}, v)$ such that*

(a) $\quad G^{\mathrm{M}}(\boldsymbol{\mu}, \triangle_c) \geq C_E(\boldsymbol{\mu}, v) > -\infty$;

(b) $\quad \mathrm{Tr}_{\mathcal{H}_{\triangle_c}} e^{-\beta(H^{\mathrm{M}}_{\triangle_c} - \boldsymbol{\mu}\cdot\boldsymbol{N})} \leq C_\Xi(\beta, \boldsymbol{\mu}, v) < \infty$,

for all $\triangle_c = \triangle \cap \Lambda_L$*, with* $L \geq L_0$ *and* $|\triangle| \leq v$*.*

For the proof of Theorem 1 we will also use the following lemma.

Lemma 6. *Let* $\{\boldsymbol{\mu}_l\}$ *be a sequence in* $\mathbb{R}^2$ *with* $\lim_{l\to\infty} \boldsymbol{\mu}_l = \boldsymbol{\mu}$ *and let* $\{\Lambda_l\}$ *be a regular sequence of domains. Then*

(a) $\quad \lim_{l\to\infty} |\Lambda_l|^{-1} G^{\mathrm{D}}(\boldsymbol{\mu}_l, \Lambda_l) = \lim_{l\to\infty} |\Lambda_l|^{-1} G^{\mathrm{D}}(\boldsymbol{\mu}, \Lambda_l) = g^{\mathrm{D}}(\boldsymbol{\mu})$ *;*

(b) $\quad \lim_{l\to\infty} p^{\mathrm{D}}(\beta, \boldsymbol{\mu}_l, \Lambda_l) = \lim_{l\to\infty} p^{\mathrm{D}}(\beta, \boldsymbol{\mu}, \Lambda_l) = p^{\mathrm{D}}(\beta, \boldsymbol{\mu})$.

Proof. We use the notation $\boldsymbol{\mu}_l = (\mu_{nl}, \mu_{kl})$ and $\boldsymbol{\epsilon} = (\epsilon, \epsilon)$. For $\epsilon > 0$, there exists an l_0 such that for all $l \geq l_0$

$$\begin{aligned} \mu_n - \epsilon \leq \quad & \mu_{nl} \quad \leq \mu_n + \epsilon \\ \mu_k - \epsilon \leq \quad & \mu_{kl} \quad \leq \mu_k + \epsilon \ . \end{aligned}$$

For (a), we note that

$$|\Lambda_l|^{-1} G^{\mathrm{D}}(\boldsymbol{\mu} + \boldsymbol{\epsilon}, \Lambda_l) \leq |\Lambda_l|^{-1} G^{\mathrm{D}}(\boldsymbol{\mu}_l, \Lambda_l) \leq |\Lambda_l|^{-1} G^{\mathrm{D}}(\boldsymbol{\mu} - \boldsymbol{\epsilon}, \Lambda_l) \ , \qquad \forall\, l \geq l_0 \ .$$

Hence

$$g^{\mathrm{D}}(\boldsymbol{\mu} + \boldsymbol{\epsilon}) \leq \liminf_{l\to\infty} |\Lambda_l|^{-1} G^{\mathrm{D}}(\boldsymbol{\mu}_l, \Lambda_l) \leq \limsup_{l\to\infty} |\Lambda_l|^{-1} G^{\mathrm{D}}(\boldsymbol{\mu}_l, \Lambda_l) \leq g^{\mathrm{D}}(\boldsymbol{\mu} - \boldsymbol{\epsilon}) \ ,$$

and, by the continuity of $\boldsymbol{\mu} \mapsto g^{\mathrm{D}}(\boldsymbol{\mu})$, (a) follows.

For (b), we first note that, by equation (2), $\boldsymbol{\mu} \mapsto p^{\mathrm{D}}(\beta, \boldsymbol{\mu})$ is convex and hence continuous. In analogy to (a) we have, using that $A \mapsto \mathrm{Tr}\, e^A$ is (operator) monotone,

$$p^{\mathrm{D}}(\beta, \boldsymbol{\mu} - \boldsymbol{\epsilon}, \Lambda_l) \leq p^{\mathrm{D}}(\beta, \boldsymbol{\mu}_l, \Lambda_l) \leq p^{\mathrm{D}}(\beta, \boldsymbol{\mu} + \boldsymbol{\epsilon}, \Lambda_l) \ , \qquad \forall\, l \geq l_0 \ .$$

Hence

$$p^{\mathrm{D}}(\beta, \boldsymbol{\mu} - \boldsymbol{\epsilon}) \leq \liminf_{l\to\infty} p^{\mathrm{D}}(\beta, \boldsymbol{\mu}_l, \Lambda_l) \leq \limsup_{l\to\infty} p^{\mathrm{D}}(\beta, \boldsymbol{\mu}_l, \Lambda_l) \leq p^{\mathrm{D}}(\beta, \boldsymbol{\mu} + \boldsymbol{\epsilon}) \ ,$$

and (b) follows by the continuity of $\boldsymbol{\mu} \mapsto p^{\mathrm{D}}(\beta, \boldsymbol{\mu})$. ☐

Proof of Theorem 1. (a) Since $H^{\mathrm{D}}_{\Lambda_L} - \boldsymbol{\mu}\cdot\boldsymbol{N} \geq H^{\mathrm{N}}_{\Lambda_L} - \boldsymbol{\mu}\cdot\boldsymbol{N}$, the inequality

$$g^{\mathrm{D}}(\boldsymbol{\mu}) \geq \limsup_{L\to\infty} g^{\mathrm{N}}(\boldsymbol{\mu}, \Lambda_L) \tag{8}$$

is obvious. We shall show the inequality $\liminf_{L\to\infty} g^{\mathrm{N}}(\boldsymbol{\mu}, \Lambda_L) \geq g^{\mathrm{D}}(\boldsymbol{\mu})$. We introduce

$$\boldsymbol{N}_{I(\Lambda)} = \int_{W\times SO(3)}^{\oplus} dy d\mu(R) \sum_{\alpha\in I(\Lambda)} \boldsymbol{N}_\alpha \ ,$$

where $\boldsymbol{N}_\alpha$ denotes the number operator of $\mathcal{H}_\alpha$. Note that $J^*\boldsymbol{N}_{I(\Lambda)}J = \boldsymbol{N}$. By Lemma 4,

$$H_\Lambda^{\mathrm{N}} - \boldsymbol{\mu}\cdot\boldsymbol{N} \geq \kappa J^* \left(H_{I(\Lambda)}^{\mathrm{N}} - \tilde{\boldsymbol{\mu}}_l \cdot \boldsymbol{N}_{I(\Lambda)}\right) J \ ,$$

where we have set $\tilde{\boldsymbol{\mu}}_l = (1/\kappa)(\boldsymbol{\mu} + l^{-1}\mathbf{const})$. We define

$$\begin{aligned} I_{y,R}^{\mathrm{int}}(\Lambda) &= \{\alpha | l\triangle_\alpha^+ \subset \Lambda^{y,R}\} \\ I_{y,R}^{\mathrm{b}}(\Lambda) &= \{\alpha | l\triangle_\alpha^+ \cap \partial\Lambda^{y,R} \neq \emptyset\} \ . \end{aligned}$$

Let $\Psi \in \mathcal{H}_{\Lambda_L}$ be normalized to one and smooth. We observe that

$$\begin{aligned} &\left(\Psi, (H_{\Lambda_L}^{\mathrm{N}} - \boldsymbol{\mu}\cdot\boldsymbol{N})\Psi\right) \\ &\geq \ \kappa \int_{W\times SO(3)} dy d\mu(R) \left(\Gamma(j_{y,R})\Psi, \sum_{\alpha\in I(\Lambda_L)} (H_{\alpha,y,R,\Lambda}^{\mathrm{M}} - \tilde{\boldsymbol{\mu}}_l\cdot\boldsymbol{N}_\alpha)\Gamma(j_{y,R})\Psi\right) \\ &\geq \ \kappa \int_{W\times SO(3)} dy d\mu(R) \left(\sum_{\alpha\in I_{y,R}^{\mathrm{int}}(\Lambda_L)} G^{\mathrm{D}}(\tilde{\boldsymbol{\mu}}_l, l\triangle_\alpha^+) + \sum_{\alpha\in I_{y,R}^{\mathrm{b}}(\Lambda_L)} G^{\mathrm{M}}(\tilde{\boldsymbol{\mu}}_l, l\triangle_\alpha^+\cap\Lambda_L^{y,R})\right) \ . \end{aligned}$$

Hence

$$\begin{aligned} &\liminf_{L\to\infty} |\Lambda_L|^{-1} G^{\mathrm{N}}(\boldsymbol{\mu},\Lambda_L) \geq \\ &\quad \liminf_{L\to\infty} \kappa \int_{W\times SO(3)} dy d\mu(R) \left(\sum_{\alpha\in I_{y,R}^{\mathrm{int}}(\Lambda_L)} \frac{|l\triangle_\alpha^+|}{|\Lambda_L|}\cdot|l\triangle_\alpha^+|^{-1}G^{\mathrm{D}}(\tilde{\boldsymbol{\mu}}_l, l\triangle_\alpha^+)\right. \\ &\qquad\qquad \left. + \sum_{\alpha\in I_{y,R}^{\mathrm{b}}(\Lambda_L)} \frac{1}{|\Lambda_L|} C_E(\tilde{\boldsymbol{\mu}}_l, |l\triangle_\alpha^+|)\right) \\ &\quad \geq \kappa(1+O(l^{-1}))\cdot|l\triangle^+|^{-1}G^{\mathrm{D}}(\tilde{\boldsymbol{\mu}}_l, l\triangle^+) \ , \end{aligned}$$

where we used that all simplices $\triangle_\alpha^+$ are congruent to a single one, which we denote by $\triangle^+$, and in the last inequality we used Lemma 5 (a) and that both limits

$$\lim_{L\to\infty} \sum_{\alpha\in I_{y,R}^{\mathrm{int}}(\Lambda_L)} \frac{|l\triangle_\alpha^+|}{|\Lambda_L|} = 1 + O(l^{-1}) \ , \tag{9}$$

$$\lim_{L\to\infty} \sum_{\alpha\in I_{y,R}^{\mathrm{b}}(\Lambda_L)} \frac{1}{|\Lambda_L|} = 0 \tag{10}$$

are uniform in $R\in SO(3)$, $y\in W$. We omit a proof of this simple facts. By Lemma 6 (a), the subsequent limit $l\to\infty$ yields

$$\liminf_{L\to\infty} g^{\mathrm{N}}(\boldsymbol{\mu},\Lambda_L) \geq g^{\mathrm{D}}(\boldsymbol{\mu}) \ . \tag{11}$$

The two inequalities (8) and (11) show the claim.

(b) The inequality

$$p^{\mathrm{D}}(\beta,\boldsymbol{\mu}) \le \limsup_{L\to\infty} p^{\mathrm{N}}(\beta,\boldsymbol{\mu},\Lambda_L) \tag{12}$$

follows from $-\Delta^{\mathrm{N}} \le -\Delta^{\mathrm{D}}$. The opposite inequality

$$\limsup_{L\to\infty} p^{\mathrm{N}}(\beta,\boldsymbol{\mu},\Lambda_L) \le p^{\mathrm{D}}(\beta,\boldsymbol{\mu})$$

is seen as follows. We set $\boldsymbol{\mu}_l = \boldsymbol{\mu} + l^{-1}\mathbf{const}$. Let $\{\varphi_i\}_{i\in I}$ be an eigenbasis of $J^*(\kappa H_{I(\Lambda_L)} - \boldsymbol{\mu}_l N_{I(\Lambda_L)})J$. Then, using Lemma 4, we have

$$\begin{aligned}
\Xi^{\mathrm{N}}(\beta,\boldsymbol{\mu},\Lambda_L) &\le \mathrm{Tr}_{\mathcal{H}_{\Lambda_L}}\, e^{-\beta J^*(\kappa H_{I(\Lambda)} - \boldsymbol{\mu}_l\cdot \boldsymbol{N}_{I(\Lambda_L)})J} \\
&= \sum_{i\in I} e^{-\beta(J\varphi_i,(\kappa H_{I(\Lambda_L)} - \boldsymbol{\mu}_l\cdot\boldsymbol{N}_{I(\Lambda_L)})J\varphi_i)} \\
&\le \sum_{i\in I}\left(J\varphi_i, e^{-\beta(\kappa H_{I(\Lambda_L)} - \boldsymbol{\mu}_l\cdot\boldsymbol{N}_{I(\Lambda_L)})} J\varphi_i\right) \\
&\le \mathrm{Tr}_{\mathcal{H}_{I(\Lambda_L)}}\, e^{-\beta(\kappa H_{I(\Lambda_L)} - \boldsymbol{\mu}_l\cdot\boldsymbol{N}_{I(\Lambda_L)})} \\
&\le \int_{W\times SO(3)} dy\, d\mu(R) \prod_{\alpha\in I^{\mathrm{int}}_{y,R}(\Lambda_L)} \mathrm{Tr}_{\mathcal{H}_\alpha}\, e^{-\beta(\kappa H^{\mathrm{D}}_\alpha - \boldsymbol{\mu}_l\cdot\boldsymbol{N}_\alpha)} \\
&\qquad \times \prod_{\alpha\in I^{\mathrm{b}}_{y,R}(\Lambda_L)} \mathrm{Tr}_{\mathcal{H}_{\alpha,y,R,\Lambda_L}}\, e^{-\beta(\kappa H^{\mathrm{M}}_{\alpha,y,R,\Lambda_L} - \boldsymbol{\mu}_l\cdot\boldsymbol{N}_\alpha)} \ ,
\end{aligned}$$

where, in the third line, we used Jensen's inequality with the spectral measure of $(\kappa H_{I(\Lambda_L)} - \boldsymbol{\mu}_l\cdot\boldsymbol{N}_{I(\Lambda_L)})$ for $J\varphi_i$. Since $0<\kappa\le 1$, we have $\kappa H^{\mathrm{D}}_\alpha \ge \kappa^2 T^{\mathrm{D}}_\alpha + \kappa V \cong H^{\mathrm{D}}_{\kappa^{-1}l\triangle^+_\alpha}$, where T^{D}_α denotes the kinetic Energy, V is the Coulomb potential, and the unitary equivalence comes from scaling. Note that all the simplices $\triangle^+_\alpha$ are congruent to a single one $\triangle^+$. By Lemma 5 (b), we have

$$\begin{aligned}
&p^{\mathrm{N}}(\beta,\boldsymbol{\mu},\Lambda_L) \\
&\quad = (\beta|\Lambda_L|)^{-1}\log \Xi^{\mathrm{N}}(\beta,\boldsymbol{\mu},\Lambda_L) \\
&\quad \le (\beta|\Lambda_L|)^{-1}\log\left(\Xi^D(\beta,\boldsymbol{\mu}_l,\kappa^{-1}l\triangle^+)^{\sup_{y,R}(|I^{\mathrm{int}}_{y,R}(\Lambda_L)|)}\cdot C_\Xi(\kappa\beta,\kappa^{-1}\boldsymbol{\mu}_l,|l\triangle^+|)^{\sup_{y,R}(|I^{\mathrm{b}}_{y,R}(\Lambda_L)|)}\right) \\
&\quad \le \sup_{y,R}(|I^{\mathrm{int}}_{y,R}(\Lambda_L)|)|\Lambda_L|^{-1}|\kappa^{-1}l\triangle^+|\cdot p^{\mathrm{D}}(\beta,\boldsymbol{\mu}_l,\kappa^{-1}l\triangle^+) \\
&\qquad\quad + \sup_{y,R}(|I^{\mathrm{b}}_{y,R}(\Lambda_L)|)(\beta|\Lambda_L|)^{-1}\cdot\log C_\Xi(\kappa\beta,\kappa^{-1}\boldsymbol{\mu}_l,|l\triangle^+|) \ ;
\end{aligned}$$

note that $\Xi^{\mathrm{D}}\ge 1$ and $C_\Xi \ge 1$. Thus

$$\limsup_{L\to\infty} p^{\mathrm{N}}(\beta,\boldsymbol{\mu},\Lambda_L) \le \kappa^{-3}(1+O(l^{-1}))p^{\mathrm{D}}(\beta,\boldsymbol{\mu}_l,\kappa^{-1}l\triangle^+) \ ,$$

where we have used equations (9, 10). Using Lemma 6 (b), the subsequent limit $l\to\infty$ gives

$$\limsup_{L\to\infty} p^{\mathrm{N}}(\beta,\boldsymbol{\mu}) \le p^{\mathrm{D}}(\beta,\boldsymbol{\mu}) \ . \tag{13}$$

The claim in (b) follows from eqns. (12) and (13). □

3.3 Proof of Lemma 5

To prove Lemma 5, we will first state a technical Lemma reflecting the geometry of Λ. We recall that $\triangle$ denotes a simplex which is similar to one of the $\triangle_\alpha$, i.e., equivalent up to dilations, translations and rotations.

Lemma 7. *Let Λ_L be a sequence of domains as in Theorem 1 and let $v > 0$. Then there exist a constant $C_\Lambda > 0$ and a number L_0 (depending on v) such that for all $L \geq L_0$ and all simplices $\triangle$ with $|\triangle| \leq v$ which intersect $\partial\Lambda_L$, we can choose an open set V containing $\triangle_c = \triangle \cap \Lambda_L$ and smooth coordinates*

$$\varphi : V \to B_0 \quad x \mapsto \varphi(x) = (y_1(x), y_2(x), y_3(x))$$

with the properties:

(i) B_0 is a ball centered around the origin and $\Lambda \cap V$ corresponds to either the half space restriction $\{x \in V \mid y_3(x) < 0\}$, the quarter space restriction $\{x \in V \mid y_2(x), y_3(x) < 0\}$, or the octant restriction $\{x \in V \mid y_1(x), y_2(x), y_3(x) < 0\}$.

(ii) The Jacobian $D\varphi$ has determinant one and $D\varphi^{-1}(D\varphi^{-1})^T \geq C_\Lambda$.

We want to point out that in the case where Λ is a box, this Lemma follows trivially by choosing $C_\Lambda = 1$ and the coordinate maps to be an appropriate composition of a translation followed by a rotation. In that case, also the next lemma is trivial.

Proof. By assumption, Λ is a bounded subset of $\mathbb{R}^3$ with smooth boundary, except for isolated edges or corners. This means that around any point $x_0 \in \partial\Lambda$ on the boundary of Λ there is an open neighborhood V_{x_0} on which we may choose smooth coordinates (y_1, y_2, y_3) such that $\Lambda \cap V_{x_0}$ corresponds to either the half space restriction $\{x \in V_{x_0} \mid y_3(x) < 0\ \}$, the quarter space restriction $\{x \in V_{x_0} \mid y_2(x), y_3(x) < 0\ \}$, or the octant restriction $\{x \in V_{x_0} \mid y_1(x), y_2(x), y_3(x) < 0\ \}$. By rescaling a coordinate we can achieve that the coordinate map φ has Jacobian determinant equal to one[1]. By possibly adjusting the coordinates and choosing the neighborhood V_{x_0} smaller, we can achieve that the images of the coordinate neighborhoods V_{x_0} under the coordinate maps are balls centered at the origin. By compactness there exist constants $C_\Lambda > 0$ and $r > 0$ such that for each point $x_0 \in \partial\Lambda$ we can choose a coordinate map $\varphi : V_{x_0} \to B$ such that

$$D\varphi^{-1}(D\varphi^{-1})^T \geq C_\Lambda$$

and moreover $|x - x_0| < r$ implies $x \in V_{x_0}$. Given such a collection of coordinate maps for Λ we obtain, by scaling, a collection of coordinate charts for Λ_L with properties *(i)*

[1]This can be achieved as follows. Let $\phi : x \mapsto w(x) = (w_1(x), w_2(x), w_3(x))$ be a coordinate map with Jacobian determinant not necessarily equal to one. Then, we define new coordinates

$$y_3(w) = \int_0^{w_3} |\det D\phi^{-1}(w_1, w_2, s)|\, ds \quad , \quad y_1 = w_1 \ , \ y_2 = w_2 \ .$$

It follows that $dy = |\det D\phi^{-1}|\, dw$ and thus the Jacobian determinant of the coordinate map $x \mapsto y(w(x))$ is 1.

and *(ii)*. Moreover, the constant r becomes Lr under this scaling. Thus for large L, $\triangle_c = \triangle \cap \Lambda_L$ is contained in some coordinate chart. $\square$

Let $-\Delta^{\mathrm{M}}_{\varphi(\triangle_c)}$ denote the Laplacian on $\varphi(\triangle_c)$ with mixed boundary conditions, i.e., φ maps Dirichlet (Neumann) boundaries of $\triangle_c$ to Dirichlet (Neumann) boundaries of $\varphi(\triangle_c)$.

Lemma 8. *Let φ be a coordinate map as in Lemma 7. Then the map $U : L^2(V) \to L^2(B_0)$ $f \mapsto f \circ \varphi^{-1}$ is unitary. Moreover, on the form domain of $-\Delta^{\mathrm{M}}_{\triangle_c}$*

$$-\Delta^{\mathrm{M}}_{\triangle_c} \geq U^* C_\Lambda (-\Delta^{\mathrm{M}}_{\varphi(\triangle_c)}) U \ .$$

Proof. Since the Jacobian determinant of φ is one, U is unitary. By abuse of notation we write $f(y)$ for $(Uf)(y) = f \circ \varphi^{-1}(y)$. We set $g^{ij} = (D\varphi^{-1}(D\varphi^{-1})^T)_{ij}$. For functions f in the form domain of $-\Delta^{\mathrm{M}}_{\triangle_c}$ we write $(f, -\Delta^{\mathrm{M}}_{\triangle_c} f)$ in terms of the y coordinates and estimate

$$\begin{aligned}
(f, -\Delta^{\mathrm{M}}_{\triangle_c} f) \quad &= \int_{\varphi(\triangle_c)} \sum_{i,j} g^{ij} \overline{\frac{\partial f}{\partial y_i}}(y) \frac{\partial f}{\partial y_j}(y)\, dy \\
&\geq \int_{\varphi(\triangle_c)} \sum_{i,j} C_\Lambda \delta^{ij} \overline{\frac{\partial f}{\partial y_i}}(y) \frac{\partial f}{\partial y_j}(y) dy \\
&= C_\Lambda (Uf, -\Delta^{\mathrm{M}}_{\varphi(\triangle_c)} Uf) \ .
\end{aligned}$$

$\square$

Lemma 9. (Lieb-Thirring estimate) *Let $v > 0$ be fixed. There exists a number L_0 and a constant C_M (depending on Λ), such that for all $L \geq L_0$ and $|\triangle| \leq v$ we have*

$$\left| \mathrm{Tr}_{L^2(\triangle_c)} (-\Delta^{\mathrm{M}}_{\triangle_c} + V)_- \right| \leq C_M \int_{\triangle_c} |V_-(x)|^{5/2}\, dx \ ,$$

where V is any locally integrable function on $\triangle_c = \triangle \cap \Lambda_L$ with negative part $V_- \in L^{5/2}$. (Note that $\mathrm{Tr}\, A_-$ denotes the trace over the negative eigenvalues of the selfadjoint operator A.)

Proof. We first observe that if $\triangle \cap \Lambda_L = \emptyset$ then the estimate is a simple consequence of the classical Lieb-Thirring inequality [7] since we have Dirichlet boundary conditions on the whole boundary. Thus for a given v let L_0 be as in Lemma 7. Assume that $\triangle$ intersects with the boundary of Λ_L and that $|\triangle| \leq v$. Let $\varphi : V \to B_0$ be a coordinate map with the properties as stated in Lemma 7. Thus $\triangle_c \in V$. We consider first the case where $V \cap \Lambda_L = \{x \in V \mid y_3(x) < 0\}$. On B_0 we define the reflection $\tau : (y_1, y_2, y_3) \mapsto (y_1, y_2, -y_3)$. By $\varphi(\triangle_c)^\tau$ we denote the interior of the closure of $\varphi(\triangle_c) \cup \tau(\varphi(\triangle_c))$. Given a function h on $\varphi(\triangle_c)$ we extend it to a function h^τ defined a.e. on $\varphi(\triangle_c)^\tau$ by setting

$$h^\tau(y) = \begin{cases} h(y)\,, & \text{if } y_3 < 0 \\ h(\tau(y))\,, & \text{if } y_3 > 0\ . \end{cases}$$

This establishes the isometric injection

$$\begin{array}{rcl} j : L^2(\varphi(\triangle_c)) & \to & L^2(\varphi(\triangle_c)^\tau) \\ f & \mapsto & 2^{-1/2} f^\tau \ . \end{array}$$

Thus for any locally integrable function W we have

$$j^*(-\Delta^{\mathrm{D}}_{\varphi(\triangle_c)^\tau} + W^\tau) j = -\Delta^{\mathrm{M}}_{\varphi(\triangle_c)} + W \ ,$$

where $-\Delta^{\mathrm{D}}_{\varphi(\triangle_c)^\tau}$ denotes the Dirichlet Laplacian on $\varphi(\triangle_c)^\tau$ w.r.t. the Euclidean metric δ^{ij}. By the Neumann condition, j maps the domain of $-\Delta^{\mathrm{M}}_{\varphi(\triangle_c)}$ into the domain of $-\Delta^{\mathrm{D}}_{\varphi(\triangle_c)^\tau}$. We then conclude using Lemma 8

$$\begin{array}{rcl} \mathrm{Tr}_{L^2(\triangle_c)}(-\Delta^{\mathrm{M}}_{\triangle_c} + V)_- & \geq & \mathrm{Tr}_{L^2(\triangle_c)}(-\Delta^{\mathrm{M}}_{\triangle_c} + V_-)_- \\ & \geq & C_\Lambda \, \mathrm{Tr}_{L^2(\varphi(\triangle_c))}(-\Delta^{\mathrm{M}}_{\varphi(\triangle_c)} + C_\Lambda^{-1} V_-)_- \\ & \geq & C_\Lambda \, \mathrm{Tr}_{L^2(\varphi(\triangle_c)^\tau)}(-\Delta^{\mathrm{D}}_{\varphi(\triangle_c)^\tau} + C_\Lambda^{-1} V_-^\tau)_- \\ & \geq & -C_\Lambda^{-3/2} C_{\mathrm{LT}} \displaystyle\int_{\varphi(\triangle_c)^\tau} |V_-^\tau(y)|^{5/2} \, dy \\ & = & -2 C_\Lambda^{-3/2} C_{\mathrm{LT}} \displaystyle\int_{\triangle_c} |V_-(x)|^{5/2} \, dx \ , \end{array}$$

where we made abuse of notation by denoting $V_- \circ \phi^{-1}$ by V_-. In the step before last we used the classical Lieb-Thirring estimate with constant C_{LT}. If $\Lambda \cap V$ has an edge or a corner the proof is essentially the same we just have to perform several reflections, which affects the value of the constant in the inequality by at most a factor 8, since in that case, we have to consider the volume obtained by reflecting $\varphi(\triangle_c)$ on all Neumann planes. Likewise we have to extend functions defined on $\varphi(\triangle_c)$. The details are left to the reader. It follows that the Lemma holds for $C_M = 16\, C_\Lambda^{-3/2} C_{\mathrm{LT}}$. □

Proof of Lemma 5. Let $\triangle$ be a simplex with $|\triangle| \leq v$. Let L_0 be sufficiently large such that the assertions of Lemmas 7 and 9 hold. Consider now $\triangle_c = \triangle \cap \Lambda_L$ for $L \geq L_0$. The Coulomb interaction is

$$\begin{array}{rcl} V_c(x_1, ..., x_n, R_1, ..., R_k) & = & \displaystyle\sum_{1 \leq i < j \leq n} \frac{1}{|x_i - x_j|} - z \sum_{i=1}^{n} \sum_{j=1}^{k} \frac{1}{|x_i - R_j|} \\ & & + z^2 \displaystyle\sum_{1 \leq i < j \leq k} \frac{1}{|R_i - R_j|} \ . \end{array}$$

We introduce the nearest neighbor, or Voronoi, cells $\{\Gamma_j\}_{j=1}^k$ defined by

$$\Gamma_j = \{ \, x \, | \, |x - R_j| \leq |x - R_l| \text{ for all } l \neq j \, \} \ .$$

Furthermore, define the distance D_j of R_j to the boundary of Γ_j, i.e.,

$$D_j = \mathrm{dist}(R_j, \partial\Gamma_j) = \frac{1}{2} \min\{|R_l - R_j|, \, j \neq l\} \ ,$$

By Theorem 6 in [8], we have the following inequality

$$V_c(x_1, ..., x_n, R_1, ..., R_k) \geq -\sum_{i=1}^{n} W(x_i) + \frac{1}{8} z^2 \sum_{j=1}^{k} D_j^{-1} , \tag{14}$$

where for x in the cell Γ_j

$$W(x) = \frac{2z+1}{|x - R_j|} .$$

We note that, in the situation considered here, the coordinates x_i and R_j all lie in $\triangle_c$. Using inequality (14), we find

$$H^{\mathrm{M}}_{\boldsymbol{N},\triangle_c} - \mu_n n - \mu_k k \geq \sum_{i=1}^{n} h_i - \mu_k k + \frac{1}{8} z^2 \sum_{j=1}^{k} D_j^{-1} ,$$

with $h_i = -\Delta^{\mathrm{M}}_{\triangle_c, x_i} - W(x_i) - \mu_n$. The fermion ground state energy of $\sum_{i=1}^{n} h_i$ is bounded below by $2\sum_j e_j$, where e_j are the negative eigenvalues of h_i. Hence by Lemma 9 ($f_+(x) = \max(f(x), 0)$)

$$\begin{aligned} & H^{\mathrm{M}}_{\boldsymbol{N},\triangle_c} - \mu_n n - \mu_k k \\ \geq \;& -2C_M \int_{\triangle_c} |(W + \mu_n)_+|^{5/2} dx - \mu_k k + \frac{1}{8} z^2 \sum_{j=1}^{k} D_j^{-1} \\ \geq \;& -2^{5/2} C_M \int_{\triangle_c} (|W|^{5/2} + |\mu_{n+}|^{5/2}) dx - \mu_k k + \frac{1}{8} z^2 \sum_{j=1}^{k} D_j^{-1} , \end{aligned} \tag{15}$$

where, for the second inequality, we have used that $(a+b)^{5/2} \leq 2^{3/2}(a^{5/2} + b^{5/2})$ for $a, b \geq 0$. We estimate the first term using

$$\begin{aligned} \int_{\triangle_c} |W|^{5/2} dx &= \sum_{j=1}^{k} \int_{\Gamma_j \cap \Delta_c} W_j(x)^{5/2} dx \\ &\leq \sum_{j=1}^{k} \int_{|x - R_j| \leq R} (2z+1)^{5/2} |x - R_j|^{-5/2} dx \\ &\quad + \sum_{j=1}^{k} \int_{\substack{x \in \Gamma_j \cap \triangle_c \\ |x - R_j| \geq R}} (2z+1)^{5/2} R^{-5/2} dx \\ &\leq (2z+1)^{5/2} (4\pi k R^{1/2} + |\triangle_c| R^{-5/2}) \\ &\leq (2z+1)^{5/2} 6 \left(\frac{4\pi}{5} \right)^{5/6} |\triangle|^{1/6} k^{5/6} , \end{aligned}$$

where we have made the optimal choice for R. To estimate the term involving the D_j, we note that for $k \geq 2$,

$$\sum_{j=1}^{k} D_j^3 \leq \lambda |\triangle| , \tag{16}$$

for some constant $\lambda > 0$. Using Hölders inequality, i.e.,

$$k = \sum_{j=1}^{k} D_j^{-3/4} D_j^{3/4} \leq \left(\sum_{j=1}^{k} D_j^{-1} \right)^{3/4} \left(\sum_{j=1}^{k} D_j^{3} \right)^{1/4} ,$$

we find

$$k^{4/3} \lambda^{-1/3} |\triangle|^{-1/3} \leq \sum_{j=1}^{k} D_j^{-1}$$

for $k \geq 2$. Inserting this into (15), we have

$$H^{\mathrm{M}}_{\boldsymbol{N},\triangle_c} - \mu_n n - \mu_k k \geq -C_1 |\triangle|^{1/6} k^{5/6} - C_2 |\triangle| |\mu_{n+}|^{5/2} - \mu_k k + C_3 |\triangle|^{-1/3} k^{4/3} (1 - \delta_{k1})$$

for some positive constants $0 < C_i < \infty$, $(i = 1, 2, 3)$, which depend only on z, and Λ. The case $k = 1$ is accounted for by $(1 - \delta_{k1})$. We minimize with respect to k with the result that

$$H^{\mathrm{M}}_{\boldsymbol{N},\triangle_c} - \mu_n n - \mu_k k \geq C_E(\boldsymbol{\mu}, v) \ , \ \forall \ \ |\triangle| \leq v \ ,$$

for some constant $C_E(\boldsymbol{\mu}, v) \in \mathbb{R}$. Hence we have shown (a).

To show (b) we decompose the kinetic energy

$$T^{\mathrm{M}}_{\triangle_c} = - \sum_{i=1}^{n} \Delta^{\mathrm{M}}_{\triangle_c, x_i} - (1/M) \sum_{j=1}^{k} \Delta^{\mathrm{M}}_{\triangle_c, R_i}$$

and use the same calculations as in (a). As a result

$$\begin{aligned} & H^{\mathrm{M}}_{\boldsymbol{N},\triangle_c} - \mu_n n - \mu_k k \\ & \quad = \frac{1}{2} T^{\mathrm{M}}_{\triangle_c} + \frac{1}{2} (T^{\mathrm{M}}_{\triangle_c} + 2V_c + 2\mu_n n + 2\mu_k k) \\ & \quad \geq \frac{1}{2} T^{\mathrm{M}}_{\triangle_c} + \phi(|\triangle|, \boldsymbol{\mu}, k) \ , \end{aligned}$$

with

$$\phi(|\triangle|, \boldsymbol{\mu}, k) := -2^{3/2} C_1 |\triangle|^{1/6} k^{5/6} + C_2 |\triangle| |2\mu_{n+}|^{5/2} - 2\mu_k k + C_3 |\triangle|^{-1/3} k^{4/3} (1 - \delta_{k1}) \ .$$

We estimate the grand canonical partition function as follows

$$\begin{aligned} \Xi^{\mathrm{M}}(\beta, \boldsymbol{\mu}, \triangle_c) &= \mathrm{Tr}_{\mathcal{H}_{\triangle_c}} \, e^{-\beta (H^{\mathrm{M}}_{\triangle_c} - \boldsymbol{\mu} \cdot \boldsymbol{N})} \\ &\leq \sum_{n=0}^{\infty} \mathrm{Tr}_{\bigwedge^n L^2(\triangle_c \times \mathbb{Z}_2)} \, e^{\beta \frac{1}{2} \sum_{i=1}^{n} \Delta^{\mathrm{M}}_{\triangle_c, x_i}} \\ & \quad \times \sum_{k=0}^{\infty} \mathrm{Tr}_{L^2(\triangle_c)^{\otimes k}} \, e^{\beta \frac{1}{2M} \sum_{j=1}^{k} \Delta^{\mathrm{M}}_{\triangle_c, R_j}} \cdot e^{-\beta \phi(\Delta, \boldsymbol{\mu}, k)} \ . \end{aligned} \tag{17}$$

If $\triangle$ does not intersect Λ_L then we have only Dirichlet boundary conditions and in this case it is known that the desired bound exists. It remains to consider the case where $\triangle$

intersects with the boundary of Λ_L. Let $\varphi : V \to B_0$ be a map with the properties as given in Lemma 7. We shall first consider the case where $V \cap \Lambda_L = \{x \in V \mid y_3(x) < 0\}$. We now use the reflection argument and the notation as introduced in the proof of Lemma 9. There we have shown that on the form domain of $-\triangle^{\mathrm{M}}_{\triangle_c}$,

$$-\Delta^{\mathrm{M}}_{\triangle_c} \geq U^* C_\Lambda (-\Delta^{\mathrm{M}}_{\varphi(\triangle_c)}) U = U^* j^* C_\Lambda (-\Delta^{\mathrm{D}}_{\varphi(\triangle_c)^\tau}) j U \ .$$

Using this estimate we find

$$\sum_{n=0}^{\infty} \mathrm{Tr}_{\bigwedge^n L^2(\triangle_c \times \mathbb{Z}_2)} e^{\beta \frac{1}{2} \sum_{i=1}^n \Delta^{\mathrm{M}}_{\triangle_c, x_i}} \leq \sum_{n=0}^{\infty} \mathrm{Tr}_{\bigwedge^n L^2(\varphi(\triangle_c)^\tau \times \mathbb{Z}_2)} e^{\beta \frac{1}{2} C_\Lambda \sum_{i=1}^n \Delta^{\mathrm{D}}_{\varphi(\triangle_c)^\tau, x_i}} \ .$$

The right hand side of this equation is the grand canonical partition function of an ideal Fermi gas with Dirichlet boundary conditions, which is known to be bounded above. Similarly we estimate

$$\begin{aligned}
\mathrm{Tr}_{L^2(\triangle_c)^{\otimes k}} e^{\beta \frac{1}{2M} \sum_{j=1}^k \Delta^{\mathrm{M}}_{\triangle_c, R_j}} &= \left(\mathrm{Tr}_{L^2(\triangle_c)} e^{\beta \frac{1}{2M} \Delta^{\mathrm{M}}_{\triangle_c}} \right)^k \\
&\leq \left(\mathrm{Tr}_{L^2(\varphi(\triangle_c)^\tau)} e^{\beta \frac{1}{2M} C_\Lambda \Delta^{\mathrm{D}}_{\varphi(\triangle_c)^\tau}} \right)^k \\
&\leq \left(\left(\frac{M}{2\pi \beta C_\Lambda} \right)^{3/2} |\varphi(\triangle_c)^\tau| \right)^k ,
\end{aligned}$$

where the last inequality follows from a standard estimate [9]. Note that $|\varphi(\triangle_c)^\tau| \leq 2|\triangle|$. We insert the above inequalities into eq. (17). The sum over k converges, due to the term with $k^{4/3}$. Thus we have shown (b) for the case where $V \cap \Lambda_L$ does not have any edges or corners. If $V \cap \Lambda_L$ has an edge or a corner the proof is essentially the same we just have to perform several reflections. We leave the details to the reader. It turns out that in the estimates above $\varphi(\triangle_c)^\tau$ is replaced by the volume obtained when reflecting $\varphi(\triangle_c)$ on all Neumann planes. Each of the three cases gives us a constant. Taking the largest we obtain the desired bound. $\square$

3.4 Proof of Theorem 3

As mentioned in Section 2, the case $\sigma \geq 0$ is trivial. Thus let $\sigma < 0$. Everything in the proof of Theorem 1 holds if we replace Neumann boundary conditions with elastic boundary conditions. The only part of the proof which does not generalize trivially to elastic boundary conditions is the proof of Lemma 5. We circumvent this by showing that the Laplacian with elastic boundary conditions can be estimated below in terms of the Laplacian with Neumann boundary conditions. We recall that $-\Delta^{\mathrm{M}}_{\triangle_c}$ is the unique self adjoint operator on $L^2(\triangle_c)$ whose quadratic form is the closure of the form $\phi \mapsto \int_{\triangle_c} |\nabla \phi|^2 \, dx$ with domain $\mathcal{D} = \{ \phi \in H^1(\triangle_c) \cap C(\overline{\triangle_c}) \mid \phi \text{ vanishes in a neighborhood of } \partial\triangle \cap \Lambda_L \}$. Let $-\Delta^{\mathrm{M},\sigma}_{\triangle_c}$ be the unique self adjoint operator on $L^2(\triangle_c)$ whose quadratic form is the closure of the form

$$\phi \mapsto \int_{\triangle_c} |\nabla \phi|^2 \, dx + \sigma \int_{\triangle \cap \partial \Lambda_L} |\phi|^2 \, dS$$

with domain $\mathcal{D}$. Below we will show that for all $\triangle_c = \triangle \cap \Lambda_L$, with $|\triangle| \le v$ and $L \ge 1$,

$$-\Delta_{\triangle_c}^{\mathrm{M},\sigma} \ge \tau(-\Delta_{\triangle_c}^{M}) - C \; , \tag{18}$$

for some τ, with $0 < \tau \le 1$, and some finite constant $C \ge 0$ depending only on σ and the geometry of Λ. Thus setting $\boldsymbol{c} = (C, C)$ we have

$$\begin{aligned} H_{\triangle_c}^{\mathrm{M},\sigma} &= T_{\triangle_c}^{\mathrm{M},\sigma} + V \\ &\ge \tau T_{\triangle_c}^{\mathrm{M}} + V - \boldsymbol{c}\cdot\boldsymbol{N} \\ &\ge \tau^{-1}(\tau^2 T_{\triangle_c}^{\mathrm{M}} + \tau V) - \boldsymbol{c}\cdot\boldsymbol{N} \\ &\cong \tau^{-1} H_{\tau^{-1}\triangle_c}^{\mathrm{M}} - \boldsymbol{c}\cdot\boldsymbol{N} \; . \end{aligned}$$

By

$$\mathrm{Tr}_{\mathcal{H}_{\triangle_c}} e^{-\beta(H_{\triangle_c}^{\mathrm{M},\sigma} - \boldsymbol{\mu}\cdot\boldsymbol{N})} \le \mathrm{Tr}_{\mathcal{H}_{\tau^{-1}\triangle_c}} e^{-\tau^{-1}\beta(H_{\tau^{-1}\triangle_c}^{\mathrm{M},\sigma} - \tau(\boldsymbol{\mu}+\boldsymbol{c})\cdot\boldsymbol{N})} \le C_{\Xi}(\tau^{-1}\beta, \tau(\boldsymbol{\mu}+\boldsymbol{c}), \tau^{-3}v)$$

it is now evident that for $\sigma < 0$ an analog of Lemma 5 for elastic boundary conditions holds.

It remains to show (18). Let

$$\begin{aligned} \xi : \overline{\Lambda} &\to \mathbb{R}^3 \\ x &\mapsto \xi(x) = (\xi_1(x), \xi_2(x), \xi_3(x)) \end{aligned}$$

be a real vector field continuously differentiable in the closed region $\overline{\Lambda}$ and satisfying the boundary condition $\boldsymbol{n}\cdot\xi \le -1$ on $\partial\Lambda$ where $\boldsymbol{n}$ denotes the inward normal. First observe that such a vector field exists. If Λ is a box or has smooth boundary this is clear. Consider now the general case, where the boundary of Λ has isolated edges and corners. Since Λ is bounded we can cover it with finitely many sufficiently small open sets V_γ, with the property that on each of these sets we can choose coordinates $x \mapsto y(x) = (y_1(x), y_2(x), y_3(x))$ such that $\Lambda \cap V_\gamma$ corresponds to either V_γ, the half space restriction $\{x \in V_\gamma \mid y_3(x) < 0\}$, the quarter space restriction $\{x \in V_\gamma \mid y_2(x), y_3(x) < 0\}$, or the octant restriction $\{x \in V_\gamma \mid y_1(x), y_2(x), y_3(x) < 0\}$, and such that there exists a vector field on V_γ which is constant in the coordinate chart and satisfies the required property on V_γ. Pasting these local vector fields together by means of a partition of unity on Λ subordinate to the open covering, we obtain a smooth vector field such that $\boldsymbol{n}\cdot\xi \le -1$. Given such a vector field on Λ, then $\xi_L(x) = \xi(x/L)$, for $L \in \mathbb{R}_+$, is a vector field on Λ_L with $\boldsymbol{n}\cdot\xi \le -1$ (here $\boldsymbol{n}$ denotes the inward normal of Λ_L). For $\phi \in H^1(\triangle_c) \cap C(\overline{\triangle}_c)$ vanishing in a neighborhood of $\partial\triangle \cap \Lambda_L$ we have

$$\int_{\triangle\cap\partial\Lambda_L} |\phi|^2 \, dS \le \int_{\triangle\cap\partial\Lambda_L} |\phi|^2 \xi_L(-\boldsymbol{n}\, dS) = \int_{\triangle_c} \nabla(\xi_L|\phi|^2)\, dx \; ,$$

where the equality follows from Gauss' Theorem. We calculate

$$\nabla(\xi_L|\phi|^2) = (\nabla\xi_L)|\phi|^2 + \xi_L(\nabla\phi^*)\phi + \xi_L\phi^*(\nabla\phi) \; ,$$

and for any $\epsilon > 0$ we have

$$|\xi_L(\nabla\phi^*)\phi + \xi_L\phi^*(\nabla\phi)| \leq \frac{1}{\epsilon}|\nabla\phi|^2 + \epsilon|\xi_L\phi|^2 \, .$$

As a result

$$\int_{\triangle\cap\partial\Lambda_L} |\phi|^2 \, dS \leq \int_{\triangle_c} \left(\frac{1}{\epsilon}|\nabla\phi|^2 + \epsilon|\xi_L\phi|^2 + |\nabla\xi_L||\phi|^2\right) dx \, .$$

This implies (18). □

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References

[1] E.H. Lieb, J.L. Lebowitz, The constitution of matter: Existence of thermodynamics for systems composed of electrons and nuclei. Advances in Math. **9**, 316–398 (1972).

[2] J.G. Conlon, E.H. Lieb, H.-T. Yau, The $N^{7/5}$ Law for Charged Bosons, Comm. Math. Phys. **116**, 417–448 (1988).

[3] G.M. Graf, D. Schenker, On the Molecular Limit of Coulomb Gases, Comm. Math. Phys. **174**, 215–227 (1995).

[4] Derek W. Robinson, Statistical mechanics of quantum mechanical particles with hard cores. I. The thermodynamic pressure. Comm. Math. Phys. **16**, 290–309 (1970)

[5] Derek W. Robinson, The thermodynamic pressure in quantum statistical mechanics. Lecture Notes in Physics, Vol. **9**, Springer–Verlag, Berlin–New York, iv+115 pp. (1971).

[6] M. Reed, B. Simon, Methods of modern mathematical physics IV: Analysis of operators, Academic Press, New York-London, (1978)

[7] E.H. Lieb, The stability of matter, Rev. Mod. Phys. *48*, 553–569 (1976).

[8] E.H. Lieb, H.-T. Yau, The Stability and Instability of Relativistic Matter, Comm. Math. Phys. **118**, 177–213 (1988).

[9] M.E. Fisher, The free energy of a macroscopic system. Arch. Rat. Mech. Anal. **17**, 337–410 (1964).